Los Alamos NATIONAL LABORATORY EST.1943

Material order independent interface reconstruction using power diagrams

S. P. Schofield, sams@lanl.gov
R. V. Garimella, rao@lanl.gov
M. M. Francois, mmfran@lanl.gov
R. Loubere, loubere@mip.ups-tlse.fr

We have developed a novel, material-order-independent method for interface reconstruction in multi-material volume-of-fluid (VOF) flow simulations. The method calculates approximate material centroids in each multi-material cell followed by a weighted Voronoi (or Power diagram) subdivision of the cell. It decomposes cells into convex, single-material subcells and matches volume fractions exactly. It works for an arbitrary number of materials on general polygonal grids and is naturally extendable to 3D.

Volume tracking or VOF methods track the volume fractions of materials in cells rather than the material interfaces themselves. When the interface in a cell is needed, it is reconstructed based on the volume fraction data. Piecewise linear interface calculation (PLIC) methods [2] calculate a normal direction for the material interface, then match a line with that normal such that it cuts off the correct volume for each material in the cell.

When a mixed cell contains $N_m > 2$ materials, PLIC methods traditionally work by separating one material from all the remaining $N_m - 1$ materials, then recalculating the volume fractions for the remaining $N_m - 1$ materials in the unused portion of the cell, and then separating the next material from the $N_m - 2$ remaining materials and so on. The result strongly depends on the order in which the materials are processed and a wrong order could lead to untimely advection of materials into neighboring cells as well as non-physical breakup of materials into little pieces.

Our power diagram method follows a new approach as shown in Figure 1. First, an approximate center of mass for each material in a cell

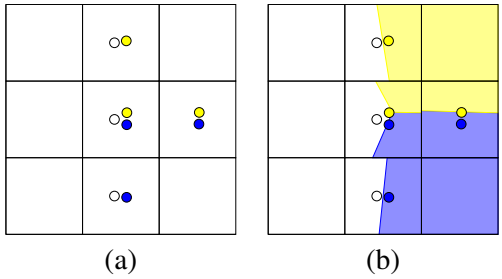

Figure 1: *Steps in new reconstruction method (a) calculate material locations from volume fractions (b) Create interface using power diagrams*

is derived from the volume fraction data. Then a *power diagram* is created using these points as generators with weights adjusted to match the volume fractions. Finally, the interface segments are smoothed with respect to their neighbors.

A power (or Laguerre) diagram is similar to a Voronoi diagram but the generators have an associated weight [1]. The Laguerre distance to a generator, $\mathbf{x_i}$, is defined as $d_L^2(\mathbf{x},\mathbf{x_i}) = d^2(\mathbf{x},\mathbf{x_i}) - \omega_i$. A power diagram cell is the set of points

$$cell((\mathbf{x_i},\omega i)) = \{\mathbf{x} \in \mathbb{R}^n | d_L^2(\mathbf{x},\mathbf{x_i}) < d_L^2(\mathbf{x},\mathbf{x_j}), \quad j = 1,\ldots,N, j \neq i\} \quad (1)$$

The weights associated with each point generator are adjusted to ensure that each power diagram cell, once clipped to the mesh cell, has the required volume fraction.

The calculation of the point generators begins by treating the volume fractions of a material like a density and calculating a linear reconstruction of the volume fraction data. The reconstruction has the form

$$\tilde{f}(\mathbf{x}) = f + \delta \cdot (\mathbf{x} - \mathbf{x_c}(\Omega)) \quad (2)$$

where δ is the volume fraction gradient and $\mathbf{x_c}$ is the centroid of the cell, Ω. A limiter on δ is used to keep $0 \leq \tilde{f}(\mathbf{x}) \leq 1$. The material locations are then calculated as the center of mass of this reconstruction.

Material order independent interface reconstruction using power diagrams

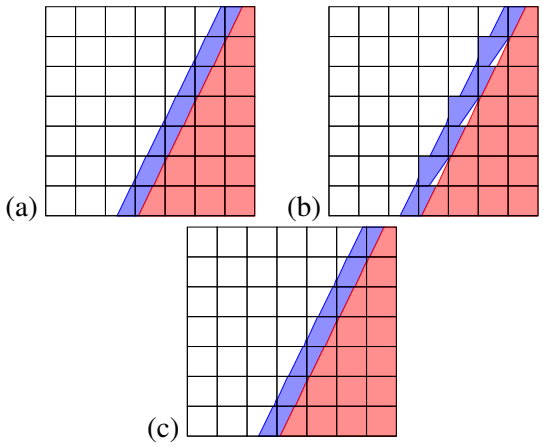

Figure 2: *Interface reconstruction of a thin filament using PLIC method with (a) correct material ordering (b) incorrect material ordering and (c) using our order-independent method*

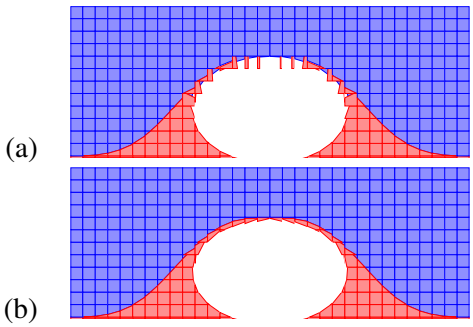

Figure 3: *Interface reconstruction of a bubble rising to a free surface using PLIC method with (a) incorrect material ordering (thin film is broken) and (b) using our order-independent method*

The interface segments are smoothed with respect to their neighbors using a constrained minimization procedure. The objective function in any cell quantifies the discrepancy between the interface segment normal and the normals of line segments joining the midpoint of this interface segment and each of its neighbors. The constraints on minimization are that volume fractions must be matched exactly and that all single-material subcells must be convex.

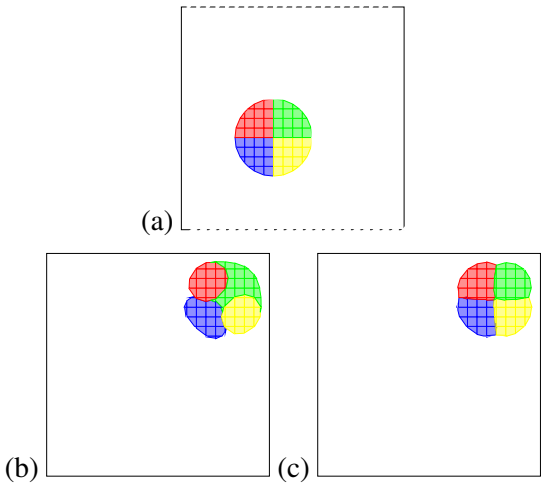

Figure 4: *Diagonal advection of a 4-material circle (a) initial state (b) final state with order-dependent method (c) with new order-independent method*

For thin filament structures such as those encountered in Rayleigh-Taylor instability calculations, an incorrect material ordering will place material on the wrong side of the filament leading to "flotsam" and "jetsam". Our material order independent, power diagram method avoids this problem as shown in Figure 2 and in Figure 3. Finally, Figure 4 shows that our method preserves a four-material junction much better than an order-dependent method in an advection test.

Current research is focused on higher order approximations to material centroids within a cell.

References

[1] F. AURENHAMMER. Power diagrams: properties, algorithms and applications. *SIAM J. Computing*, 16(1):78–96, 1987.

[2] W. J. RIDER AND D. B. KOTHE. Reconstructing volume tracking. *J. of Comp. Phys.*, 141:112–152, 1998.

Acknowledgements

This work was carried out under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396, and supported by the Advanced Simulation and Computing Program.

Los Alamos Report LA-UR-07-0587.

http://math.lanl.gov/, T-7, MS B284, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545